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Calculation of Displacement per Atom (DPA) in STREAM

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1. Introduction

The DPA value (Displacement per Atom) indicates the defects in crystal solid that are created by incident neutron interacting with material, which is an important assessment for materials strength studies of nuclear reactor components under irradiation [1]. Recently, an effort has been made to introduce the DPA calculation capability in STREAM.

STREAM developed by the Computational Reactor Physics and Experiment Laboratory (CORE) at the Ulsan National Institute of Science and Technology (UNIST) is a deterministic neutron-transport code specialized for the analysis of two-dimensional or three-dimensional reactor cores [2]. The generation of a multigroup damage cross section library and the DPA calculation steps in STREAM are presented in this paper.

2. Method and Results

2.1. DPA calculation method

The number of dislocated atoms (DA) in a crystalline solid by neutron irradiation is calculated by Eq. (1) (as in NRT model [3,4]).

$$\boldsymbol{DA} = \boldsymbol{\eta} \sum_{i=1}^{nuclide} \frac{\boldsymbol{E_i^A}}{\boldsymbol{2E_i^D}} \quad (1)$$

where the sum with the index *i* is over all the different nuclide in the interested material. The term $\boldsymbol{E_i^A}$ represents the available energy of nuclide *i* to form the atomic displacements, $\boldsymbol{E_i^D}$ is the displacement threshold (energy to dislocate an atom) of *i* and $\boldsymbol{\eta}$ is an efficiency factor, usually set as 80%.

The value $\boldsymbol{E_i^D}$ is nuclide dependence and material dependence. Some typical values of $\boldsymbol{E_i^D}$ are shown in Table I [5]. If the $\boldsymbol{E_i^D}$ for a certain nuclide is not given, STREAM adapts a value of 25 eV as a rough estimation in the calculation. The $\boldsymbol{E_i^A}$ value for a certain nuclide is computed as:

$$\boldsymbol{E_i^A = \phi N_i \sigma_{da} V} \quad (2)$$

where $\boldsymbol{\phi}$ is the neutron flux (#/cm^2-s), $\boldsymbol{N_i}$ is the number density (#/barn-cm), $\boldsymbol{\sigma_{da}}$ is the damage cross section (eV-barn) and V is the material volume (cm^3).

The DPA rate (per second) is then simply obtained by dividing the DA value by the total number of atoms in the interested material.

$$\boldsymbol{DPA} = \frac{\boldsymbol{DA}}{\boldsymbol{V \times \sum_{i=1}^{nuclide} N_i \times 10^{24}}} \quad (3)$$

The generation of damage cross section and verification of DPA calculation in STREAM are presented in the next sections.

Table I. $\boldsymbol{E_i^D}$ of some typical elements in materials.

Element	E_D (eV)	Element	E_D (eV)
Zr	40	ZnO	40 (Zn) 57 (O)
Fe	17-44	ZnS	10 (Zn) 15 (S)
UO_2	40 (U) 20 (O)	C graphite	28-31
Al	19-27	C diamond	80

2.2. Damage cross section

The damage micro cross section is generated from ENDF/B-VII.1 library [6] by nuclear data processing code NJOY [7]. The HEATR module in NJOY will be called to generate the damage cross section (MT=444). To be consistent with the damage cross section used in MCS [8] or MCNP (ACE format) [9], the tag for gamma transport is turned on in HEATR so that the energy of gamma generated from neutron induced reactions do not contribute to the damage energy. The comparison of multigroup damage cross section with the continuous one for some common nuclides in nuclear reactors is shown in Fig. 1.

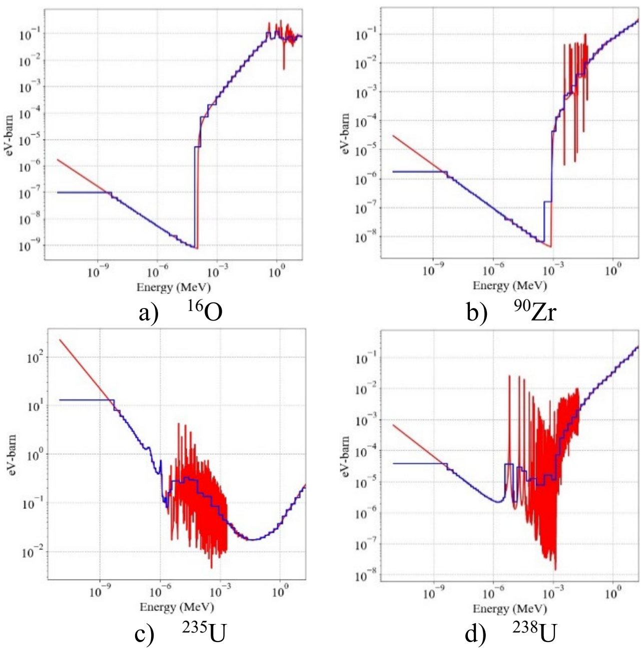

Figure 1. Multigroup damage cross section for STREAM (blue) compared to damage cross section for MCS (red).

Good agreement is observed between the generated multigroup damage cross section for STREAM (in 72 groups format) compared to the data used for MCS/MCNP.

2.3. DPA comparison to MCS

MCS is a Monte Carlo code that has been developed at the Ulsan National Institute of Science and Technology. The DPA calculation based on NRT model has been implemented in MCS and has been verified against MCNP [8]. Thus, the DPA from STREAM is compared to MCS for a VERA 1B pin cell problem [10]. The configuration of this pin cell is shown in Fig. 2.

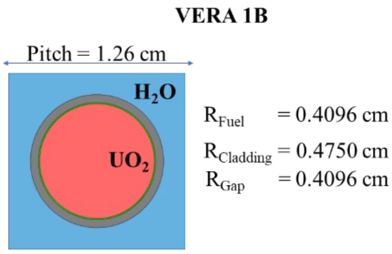

Figure 2. Configuration of the VERA 1B pin cell.

Power density is set as 40 W/g and the depletion was run up to a final burnup of 80 MWd/kg. STREAM results for DPA in fuel and cladding region are shown in Fig. 3, comprising the accumulated DPA and the DPA rate (per year).

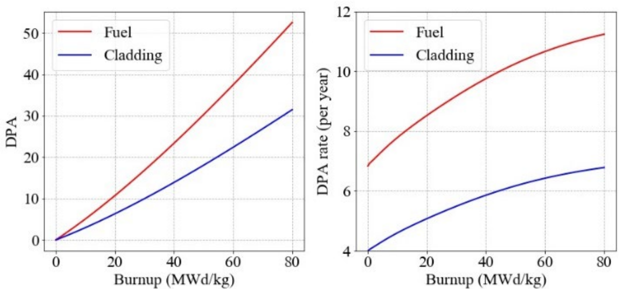

Figure 3. DPA results from STREAM for fuel and cladding.

The number densities of fuel at three burnup steps are copied from STREAM and used in MCS to ensure consistency. In addition, if the $\boldsymbol{E_i^D}$ values are not available for a certain nuclide, 25 eV is used for both codes. Comparison to MCS at BOC (0 MWd/kg), MOC (40 MWd/kg) and EOC (80 MWd/kg) is shown in Table II: Relative error of MCS is ~ 10^{-3} and is not shown.

Table II. DPA rate (DPA/year) in fuel and cladding in comparison to MCS.

	Fuel	STREAM/ MCS-1 (%)	Cladding	STREAM/ MCS-1 (%)
BOC	6.62	1.09	3.86	0.42
MOC	9.48	0.70	5.62	0.46
EOC	10.59	0.51	6.23	0.32

The DPA calculation in STREAM shown good agreement to MCS.

3. Conclusion

The multigroup damage cross section is generated for STREAM by NJOY (MT=444). The DPA calculation is based on the NRT model and good agreement is observed when compared to MCS. The DPA calculation in STREAM has extended the code's capabilities to estimate the radiation damage to the reactor materials and components.

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